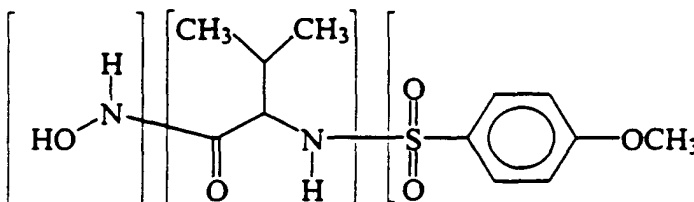
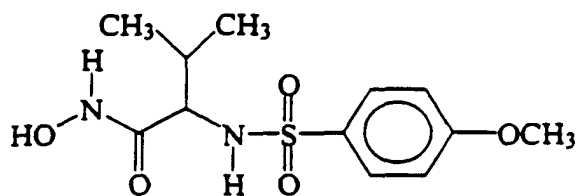


# Compound CI



	Fi	Fii	Fiii
Molecular formula	$H_2NO$	$C_5H_9NO$	$C_7H_7O_3S$

Figure 1

09753869, 041601

APPROVED	O.G. FIG.	
BY	CLASS	SUBCLASS
DRAFTSMAN		

Pocket No.: IBIS-0339  
 Title: GENERATION OF VIRTUAL COMBINATORIAL  
 LIBRARIES OF COMPOUNDS  
 Inventors: Richard Griffey and Eric Swayze  
 Atty: Paul K. Legaard - Telephone: 215 568 3100

Sheet 2 of 20

### Addition of fragments to yield compounds

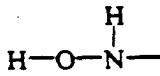
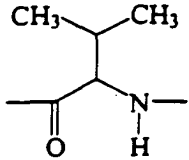
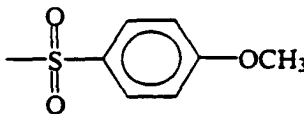
Fragment Identifier	Table			
	Structure	Name	Molecular formula	Other
F <sub>i</sub>		Hydroxylamine	H <sub>2</sub> NO	...
F <sub>ii</sub>		Amino acid	C <sub>5</sub> H <sub>9</sub> NO	...
F <sub>iii</sub>		Sulfonyl	C <sub>7</sub> H <sub>7</sub> O <sub>3</sub> S	...

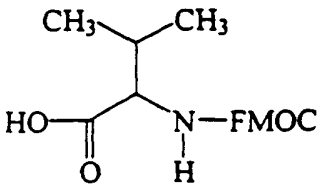
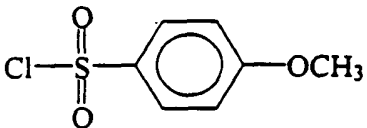
Figure 2

09753859-041601

APPROVED	O.G. FIG.	
BY	CLASS	SUBCLASS
DRAFTSMAN		

Docket No.: IBIS-0339  
 Title: GENERATION OF VIRTUAL COMBINATOR  
 LIBRARIES OF COMPOUNDS  
 Inventors: Richard Griffey and Eric Swayze  
 Atty: Paul K. Legaard - Telephone: 215 568 3100

Sheet 3 of 20

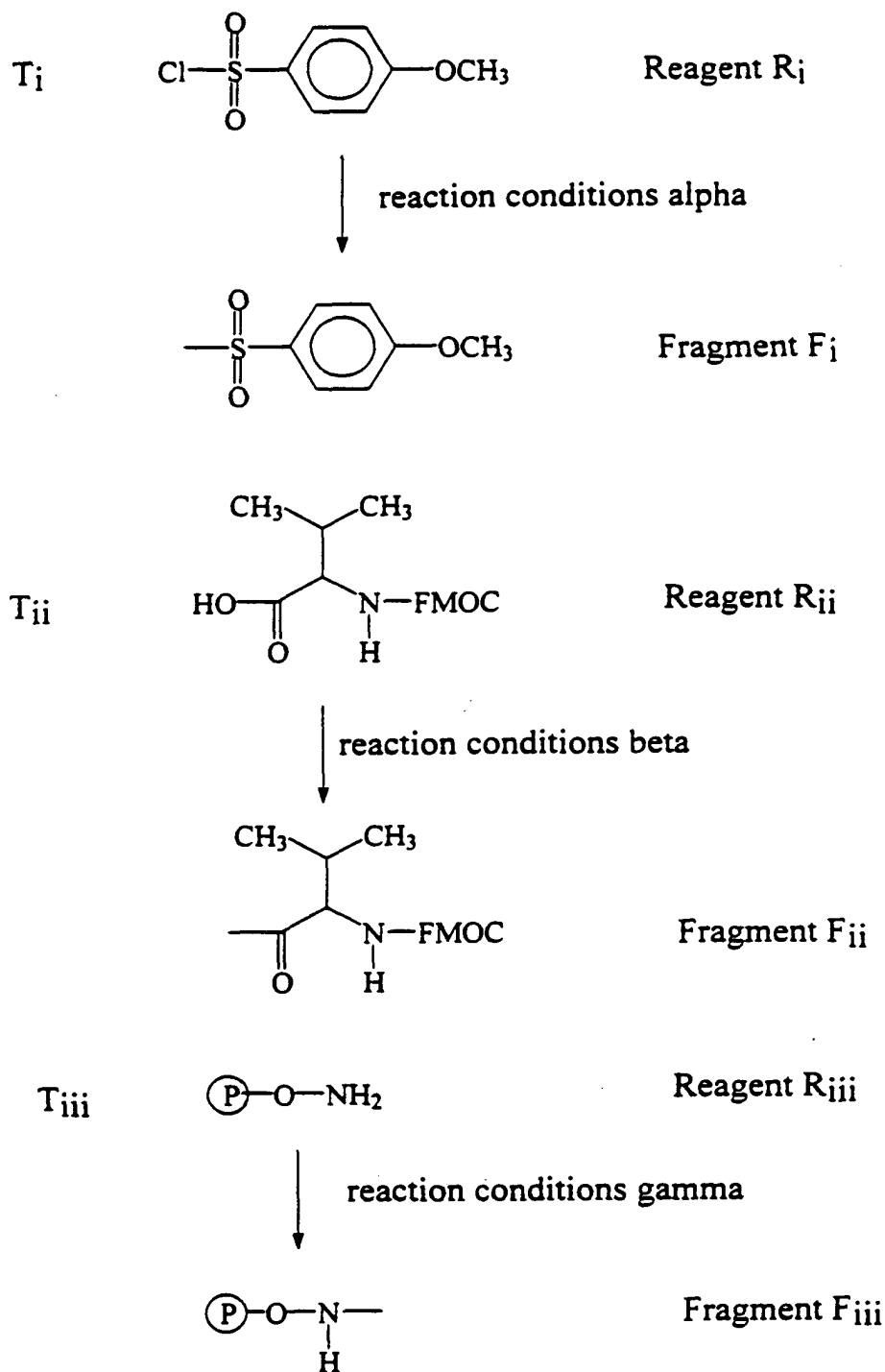
Reagents	Identifier	Name	Properties
$\text{H}-\text{O}-\text{NH}_2$ or $\text{(P)}-\text{O}-\text{NH}_2$	R <sub>i</sub>	Hydroxylamine	...
	R <sub>ii</sub>	Fmoc blocked amino acid	...
	R <sub>iii</sub>	Sulfonylchloride	...

$\text{(P)}$  = Solid support

Figure 3

09753069.041504  
 T09T70" 6905260

# Transformation



Ⓟ = Solid support

Figure 4

09753869, 041601

APPROVED	O.C. FIG.
BY	CLASS/SUBCLASS
DRAFTSMAN	

Patent No.: IBIS-0339  
 GENERATION OF VIRTUAL COMBINATORIAL  
 LIBRARIES OF COMPOUNDS  
 Inventors: Richard Griffey and Eric Swayze  
 Atty: Paul K. Legaard - Telephone: 215 568 3100

Sheet 5 of 20

## Common Fragment / Different Reagents and Transformations

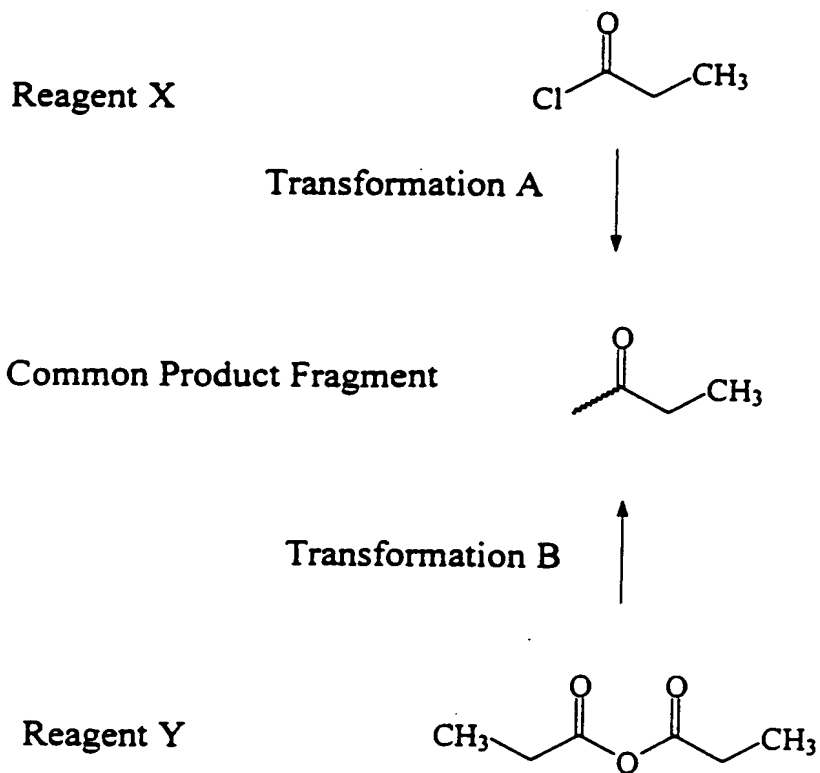


Figure 5

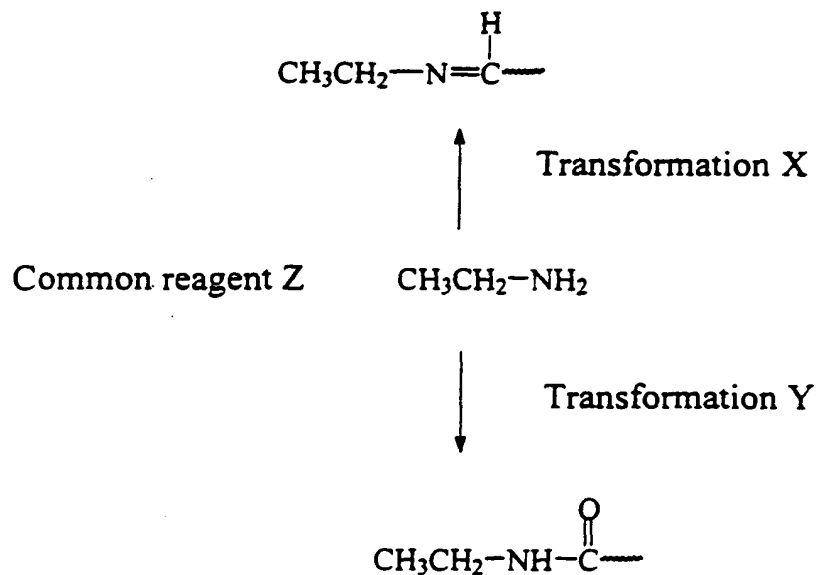
09753869 041601

APPROVED	O.G. FIG.
BY	CLASS/RECLASS
DRAFTSMAN	

Patent No.: IBIS-0339  
 GENERATION OF VIRTUAL COMBINATORIAL  
 LIBRARIES OF COMPOUNDS  
 Inventors: Richard Griffey and Eric Swayze  
 Atty: Paul K. Legaard - Telephone: 215 568 3100

Sheet 6 of 20

## Common Fragment / Different Reagents and Transformations



09753869-041604

Figure 6a

APPROVED	O.G. FIG.
BY	CLASS SUBCLASS
DRAFTSMAN	

Docket No.: IBIS-0339  
 Title: GENERATION OF VIRTUAL COMBINATO  
 LIBRARIES OF COMPOUNDS  
 Inventors: Richard Griffey and Eric Swayze  
 Atty: Paul K. Legaard - Telephone: 215 568 3100

Sheet 7 of 20

## Common Reagent

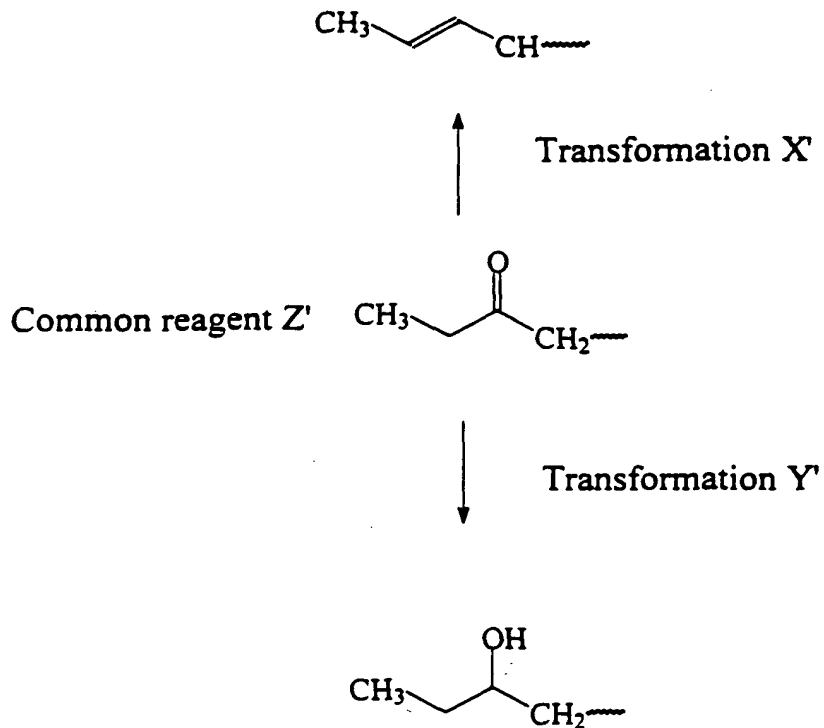


Figure 6b

09753869, 04-16-01

APPROVED	O.G. FIG.	
BY	CLASS	SUBCLASS
DRAFTSMAN		

# Symbolic addition of fragments to yield compound

<u>Symbolic Structure</u>	<u>Symbolic Identifier</u>	<u>Molecular formula</u>
---------------------------	----------------------------	--------------------------

## Fragment



$F_i$

$C_uH_vN_w \dots$



$F_{ii}$

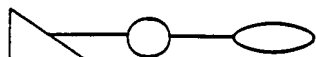
$C_uH_vN_w \dots$



$F_{iii}$

$C_uH_vN_w \dots$

## Compound



$CI$

$C_uH_vN_w \dots$

Molecular formula  $F_i$

+

Molecular formula  $F_{ii}$

+

Molecular formula  $F_{iii}$

= Molecular formula  $CI$

Figure 7

09753869-041604



APPROVED	O.G. FIG.	
BY	CLASS	SUBCLASS
DRAFTSMAN		

Project No.: IBIS-0339  
 Title: GENERATION OF VIRTUAL COMBINATORIAL  
 LIBRARIES OF COMPOUNDS  
 Inventors: Richard Griffey and Eric Swayze  
 Atty: Paul K. Legaard - Telephone: 215 568 3100

Sheet 9 of 20

## Symbolic Reagent Table

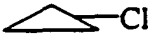
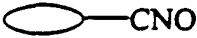

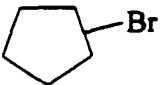
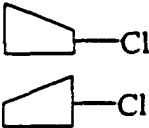



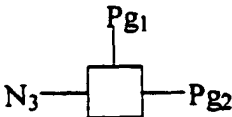
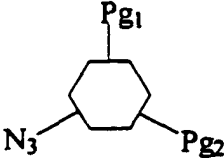
<u>Identifier</u>	<u>Name</u>	<u>Structure</u>	<u>Molecular formula</u>
R1	xxx		xxx
R2	...		...
R3	...		...
R4	...		...
R5	...		...
R6	...		...
R7	...		...
R8	...		...
R9	...		...
R10	...		...

Figure 8

09753869 041601

APPROVED	O.G. FIG.	
BY	CLASS	SUBCLASS
DRAFTSMAN		

Packet No.: IBIS-0339  
 : GENERATION OF VIRTUAL COMBINATORIA  
 RARIES OF COMPOUNDS  
 Inventors: Richard Griffey and Eric Swayze  
 Atty: Paul K. Legaard - Telephone: 215 568 3100

Sheet 10 of 20

## Symbolic Fragment Table




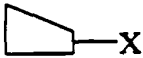
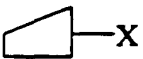


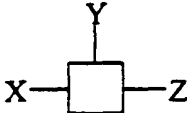
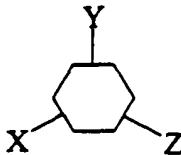
<u>Identifier</u>	<u>Symbolic Structure</u>	<u>Molecular formula</u>	<u>Molecular Weight</u>
F1		xxx	xxx
F2		...	...
F3		...	...
F4	 	...	...
F5		...	...
F6		...	...
F7		...	...
F8		...	...

Figure 9

09753869-041604  
T09T40" 698E5260

APPROVED	O.G. FIG.	
BY	CLASS	SUBCLASS
DRAFTSMAN		

## Symbolic Transformation Table





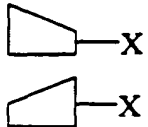



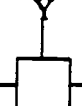
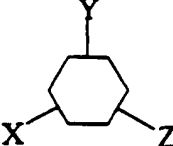
Identifier		Symbolic Reactions	Reagent
T1	F1	 ← R1	conditions α
T2	F2	 ← R2	conditions β
T3	F3	 ← R3	conditions α
T4	F3	 ← R4	conditions α
T5	F4	 ← R5	conditions α
T6	F5	X—  —Y ← R6	conditions ε
T7	F5	X—  —Y ← R7	conditions α
T8	F6	X—  —Y ← R8	conditions α
T9	F7	X—  —Z ← R9	conditions γ
T10	F8	X—  ← R10	conditions γ

Figure 10

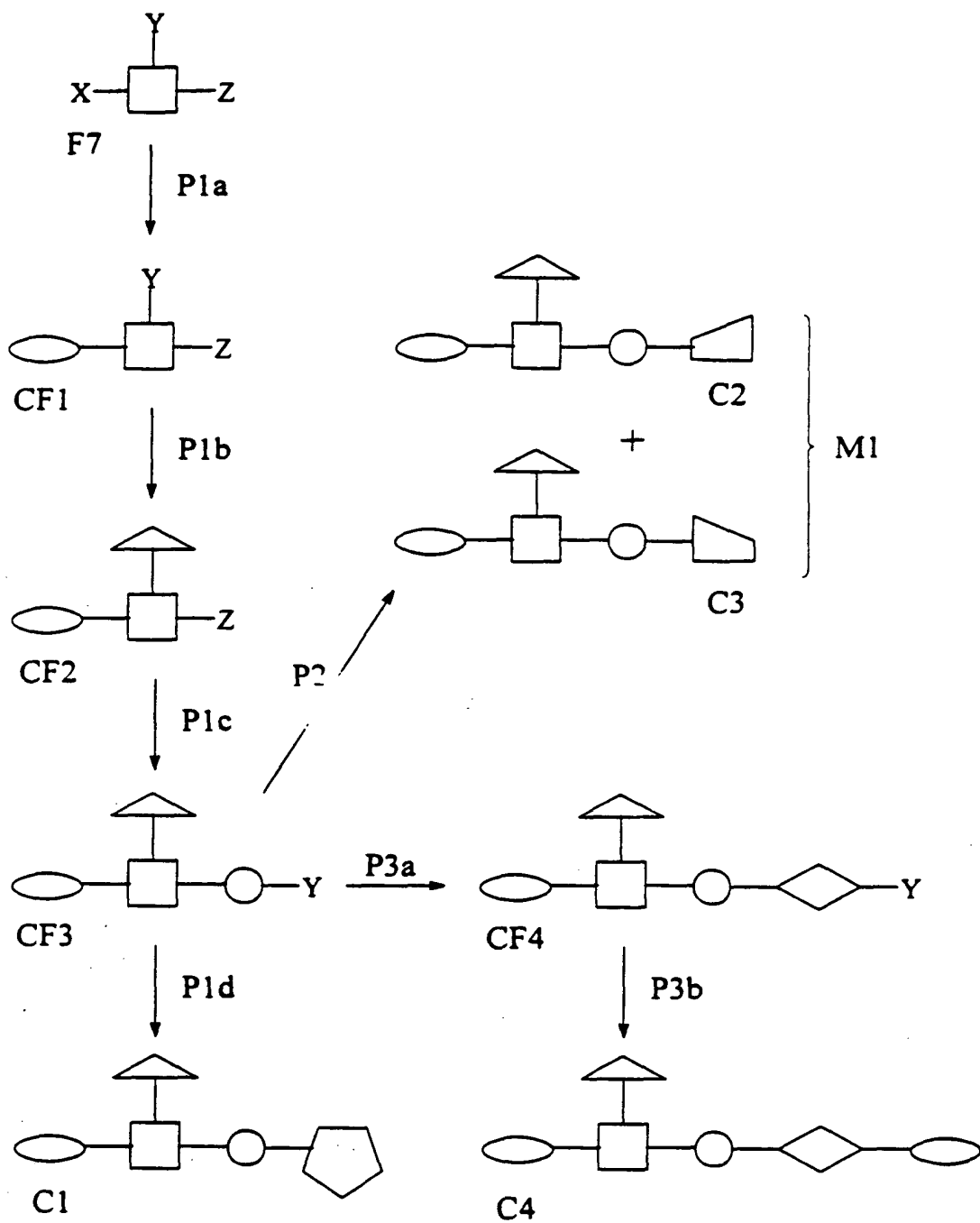
09753869.041601

APPROVED	O.G. FIG.	
BY	CLASS	SUBCLASS
DRAFTSMAN		

Docket No.: IBIS-0339  
 GENERATION OF VIRTUAL COMBINATORIAL  
 LIBRARIES OF COMPOUNDS  
 Inventors: Richard Griffey and Eric Swayze  
 Atty: Paul K. Legaard - Telephone: 215 568 3100

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## Single Compounds and Mixtures



P = synthetic path    CF = complex fragment  
 F = fragment        M = mixture  
 C = compound

Figure 11

09753869.041603

APPROVED	O.G. FIG.	
BY	CLASS	SUBCLASS
DRAFTSMAN		

Docket No.: IBIS-0339  
Title: GENERATION OF VIRTUAL COMBINATO  
LIBRARIES OF COMPOUNDS  
Inventors: Richard Griffey and Eric Swayze  
Atty: Paul K. Legaard - Telephone: 215 568 3100

Sheet 13 of 20

## Mixture 2

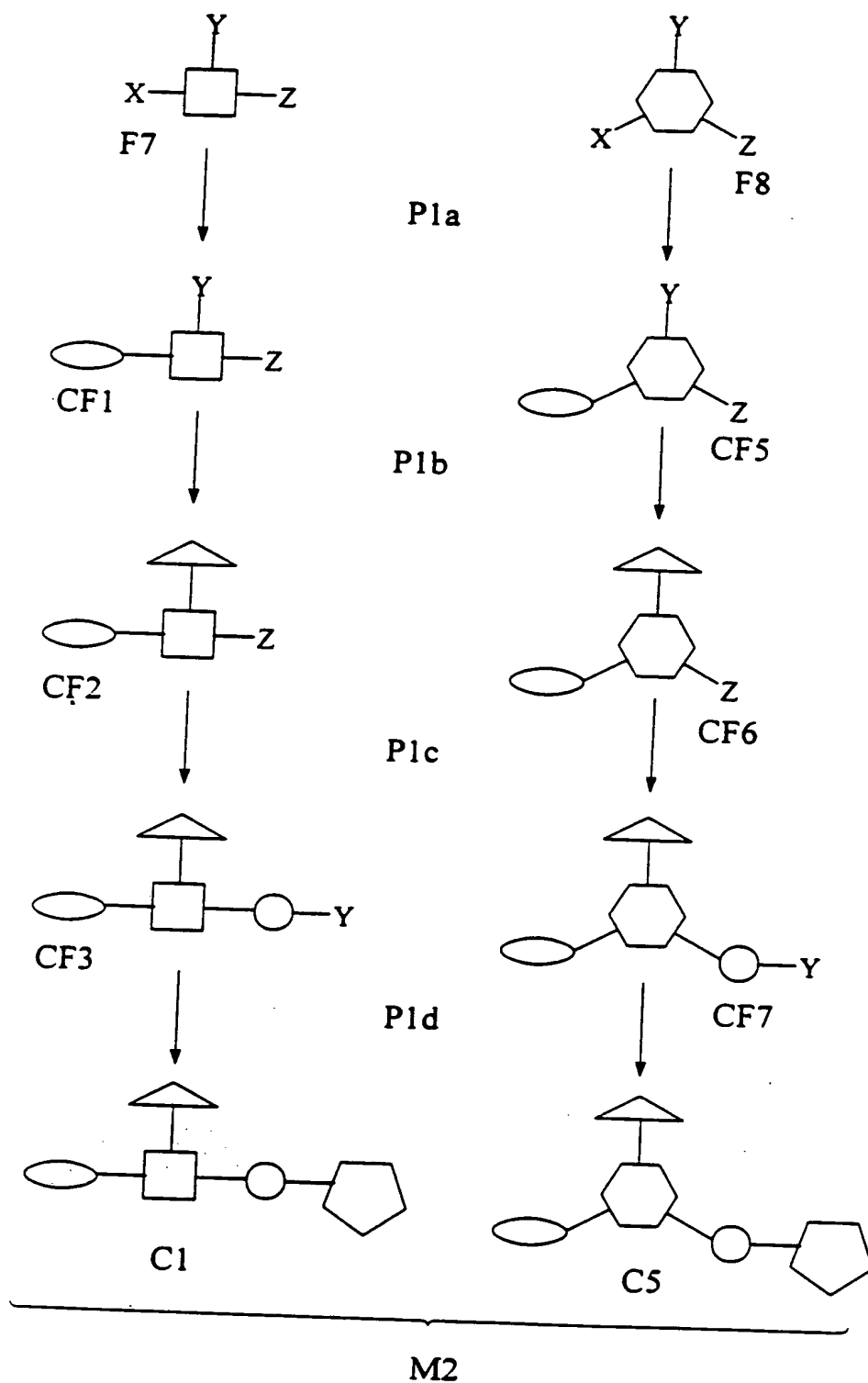


Figure 12

09753869 041601

### Mixture 3

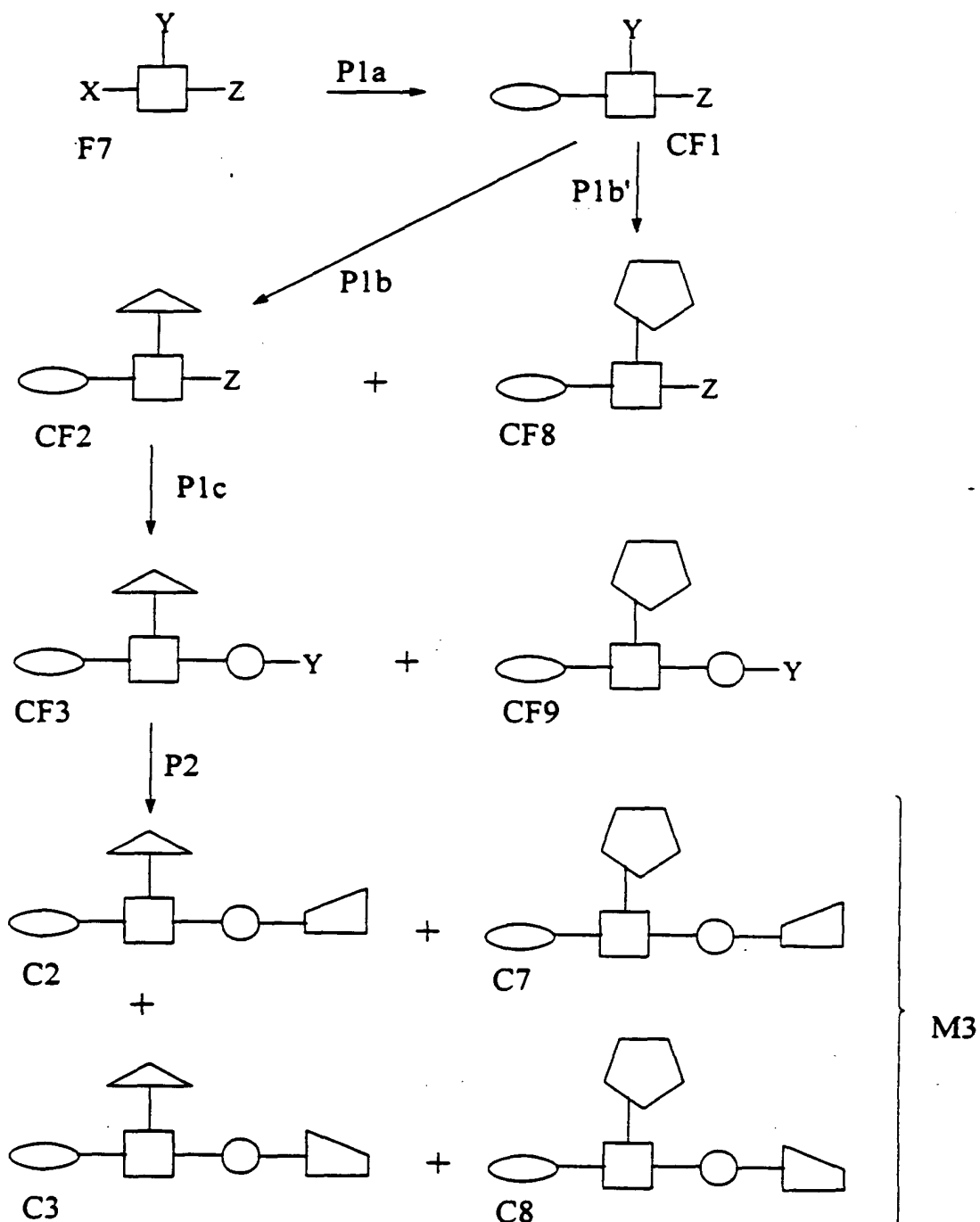


Figure 13

09753369.041601

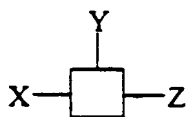
APPROVED	O.G. FIG.
BY	CLASS SUBCLASS
DRAFTSMAN	

Doc. No.: IBIS-0339  
 TITLE: GENERATION OF VIRTUAL COMBINATORIAL  
 LIBRARIES OF COMPOUNDS  
 Inventors: Richard Griffey and Eric Swayze  
 Atty: Paul K. Legaard - Telephone: 215 568 3100

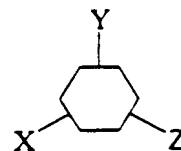
Sheet 15 of 20

## Mixture 4

### 2 Starting Fragments

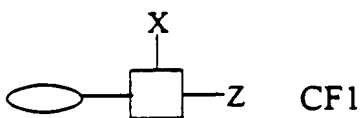


F7

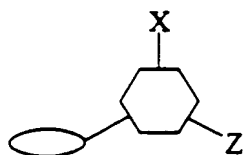


F8

### 2 Complex Fragments

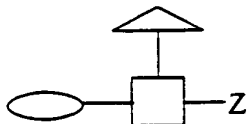


CF1

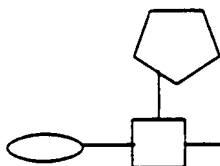


CF5

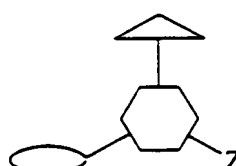
### 4 Complex Fragments



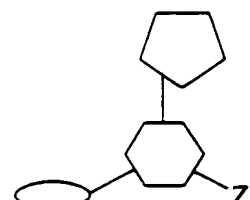
CF2



CF8

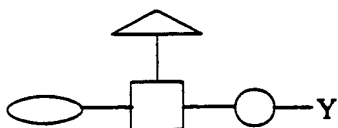


CF 6

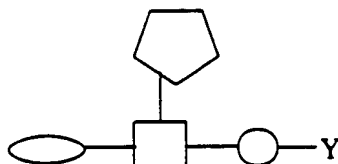


CF11

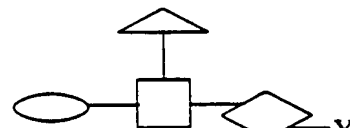
### 8 Complex Fragments



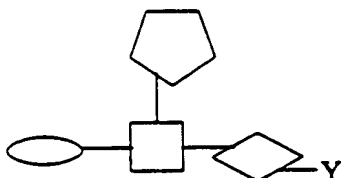
CF3



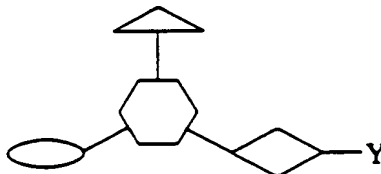
CF9



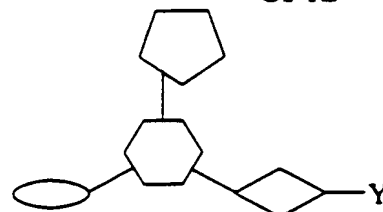
CF12



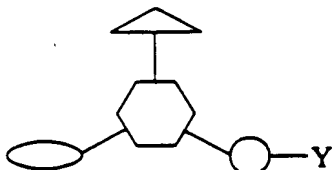
CF13



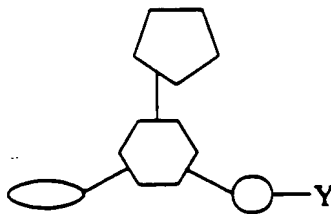
CF15



CF16



CF 7



CF14

Figure 14a

09753869.04.1601  
 109140" 698E5260

# Mixture 4 (continued)

## 16 compounds

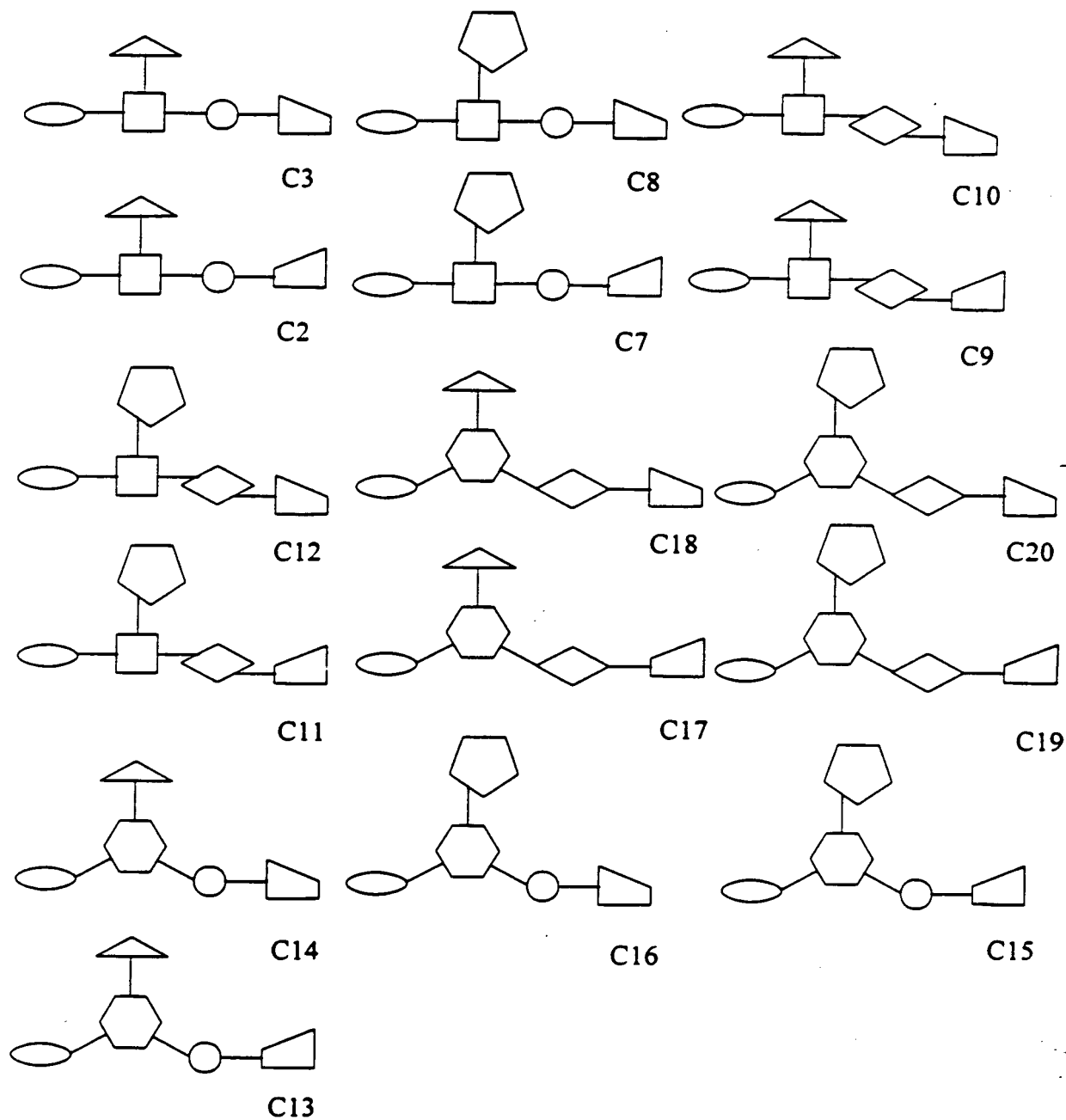


Figure 14b



APPROVED	O.G. FIG.	
BY	CLASS	SUBCLASS
DRAFTSMAN		

Pat No.: IBIS-0339  
 GENERATION OF VIRTUAL COMBINATORIAL  
 LIBRARIES OF COMPOUNDS  
 Inventors: Richard Griffey and Eric Swayze  
 Atty: Paul K. Legaard - Telephone: 215 568 3100

Sheet 17 of 20

## Tracking Table for Compound C1

### (a) By Fragments:

n	n+1	n+2
F7	F2 F1 F5	F3

### (b) By Transformations:

#### Synthesis Path 1

n	n+1	n+2
T9	T2 T1 T6	T3

#### Synthesis Path 2

n	n+1	n+2
T9	T2 T1 T7	T3

#### Synthesis Path 3

n	n+1	n+2
T9	T2 T1 T6	T4

#### Synthesis Path 4

n	n+1	n+2
T9	T2 T1 T7	T4

Figure 15

09753869 041601

APPROVED	O.G. FIG.	
BY	CLASS	SUBCLASS
DRAFTSMAN		

Docket No.: IBIS-0339  
 Title: GENERATION OF VIRTUAL COMBINATORIAL  
 LIBRARIES OF COMPOUNDS  
 Inventors: Richard Griffey and Eric Swayze  
 Atty: Paul K. Legaard - Telephone: 215 568 3100

Sheet 18 of 20

## Tracking Table

### Tracking M1

#### Step 1

T9		
----	--	--

#### Step 2

T9	T2	
----	----	--

#### Step 3

T9	T2 T1	
----	----------	--

#### Step 4

T9	T2 T1 T7	
----	----------------	--

#### Step 5

T9	T2 T1 T7	T5 <sup>1</sup>
----	----------------	-----------------

C2

#### Step 5

T9	T2 T1 T7	T5 <sup>2</sup>
----	----------------	-----------------

C3

Figure 16

09753869-041501

APPROVED	O.G. FIG.	
BY	CLASS	SUBCLASS
DRAFTSMAN		

Patent No.: IBIS-0339  
 GENERATION OF VIRTUAL COMBINATORIAL  
 LIBRARIES OF COMPOUNDS  
 Inventors: Richard Griffey and Eric Swayze  
 Atty: Paul K. Legaard - Telephone: 215 568 3100

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## Tracking Table

### Tracking M2

**Step 1**

n	n+1	n+2
T9		

**Step 1**

n	n+1	n+2
T10		

**Step 2**

n	n+1	n+2
T9	T2	

**Step 2**

n	n+1	n+2
T10	T2	

**Step 3**

n	n+1	n+2
T9	T2 T1	

**Step 3**

n	n+1	n+2
T10	T2 T1	

**Step 4**

n	n+1	n+2
T9	T2 T1 T7	

**Step 4**

n	n+1	n+2
T10	T2 T1 T7	

**Step 5**

n	n+1	n+2
T9	T2 T1 T7	T4

**Step 5**

n	n+1	n+2
T10	T2 T1 T7	T4

C1

C5

Figure 17

09753869.042601

APPROVED	O.G. FIG.	
BY	CLASS	SUBCLASS
DRAFTSMAN		

Docket No.: IBIS-0339  
 Title: GENERATION OF VIRTUAL COMBINATORIAL  
 LIBRARIES OF COMPOUNDS  
 Inventors: Richard Griffey and Eric Swayze  
 Atty: Paul K. Legaard - Telephone: 215 568 3100

Sheet 20 of 20

## Tracking Table

### Tracking M3

#### Step 1

T9		
----	--	--

#### Step 2

T9	T2	
----	----	--

#### Step 3

T9	T2 T1	
----	----------	--

#### Step 3

T9	T2 T3	
----	----------	--

#### Step 4

T9	T2 T1 T7	
----	----------------	--

#### Step 4

T9	T2 T3 T7	
----	----------------	--

#### Step 5

T9	T2 T1 T7	
----	----------------	--

C2

#### Step 5

T9	T2 T1 T7	
----	----------------	--

C3

#### Step 5

T9	T2 T3 T7	
----	----------------	--

C7

#### Step 5

T9	T2 T3 T7	
----	----------------	--

C8

Figure 18

09753069 041601